INTISARI

PERAN KATION ORGANIK PADA KARAKTERISTIK ELEKTRONIK DAN STRUKTUR SPIN HYBRID ORGANIC-INORGANIC PEROVSKITES $CH_3NH_3PbX_3$: KAJIAN TEORETIK DAN KOMPUTASIONAL BERDASARKAN PENDEKATAN DENSITY FUNCTIONAL THEORY

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Perhitungan struktur elektronik dan spin telah dilakukan dengan menggunakan Density Functional Theory (DFT) untuk Hybrid Organic-Inorganic Perovskite (HOIP) $CH_3NH_3PbX_3$ (X = I, Br, Cl). Pada penelitian ini, senyawa tersebut ditinjau pada fase suhu tinggi dari sistem bulk, yang mana peran dari kation organik ditinjau di dalam struktur kristal kubik. Orientasi kation khusus yang diposisikan di sepanjang arah $[111]$, $[101]$ dan $[011]$ juga diuji di unit sel. Perhitungan DFT untuk struktur elektronik menunjukkan bahwa orientasi $[011]$ memunculkan karakteristik celah pita *indirect*, sementara orientasi $[101]$ dan $[111]$ memunculkan celah pita *direct*. Selain itu, kemunculan pemecahan spin anisotropik yang besar juga ditemukan berturut-turut, untuk arah $[011]$, $[101]$ dan $[111]$. Perhitungan polarisasi spin mengungkapkan perbedaan karakteristik tekstur spin untuk tiap orientasi. Pada kasus $[111]$ dan $[101]$ berturut-turut, efek Rashba teridentifikasi dengan komponen *out-of-plane* sementara efek Rashba-Dresselhaus juga teridentifikasi dengan komponen *out-of-plane* yang mana tekstur spin didominasi oleh efek Dresselhaus. Pada orientasi $[011]$, efek baru yang memiliki komponen *unidirectional out-of plane* dapat diperoleh yang disebut sebagai keadaan *Persistent Spin Helix* (PSH). Untuk menyelidiki karakteristik pemecahan spin anisotropik untuk tiap orientasi kation organik, Hamiltonian efektif dari analisis teoretik grup dan tinjauan simetri dirumuskan berdasarkan pada teori $\vec{k} \cdot \vec{p}$ *perturbation*. Kemudian, kekuatan spin orbit dari ketiga efek tersebut dihitung dan model tekstur spin untuk tiap orientasi juga dideskripsikan dengan grup titik C_{3v} and C_s. Penemuan tersebut menunjukkan bahwa fase suhu tinggi dari sistem bulk HOIP $CH_3NH_3PbX_3$ merupakan material menjanjikan untuk pengembangan piranti spintronik berbasis perovskite.

Kata-kata kunci :Hybrid Organic-Inorganic Perovskite (HOIP), Efek Rashba-Dresselhaus, Persistent Spin Helix, Interaksi Spin-Orbit, Density Functional Theory, Teori gangguan $\boldsymbol{k \cdot p}$, Spintronik

ABSTRACT

THE ROLE OF ORGANIC CATION ON THE ELECTRONIC PROPERTIES AND SPIN STRUCTURES OF THE HYBRID ORGANIC-INORGANIC PEROVSKITES $CH_3NH_3PbX_3$: THEORETICAL AND COMPUTATIONAL STUDIES BASED ON DENSITY FUNCTIONAL THEORY

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It has been conducted both of the calculation of electronic and spin structure using Density Functional Theory (DFT) for the Hybrid Organic-Inorganic Perovskites (HOIP) $CH_3NH_3PbX_3$ (X = I, Br, Cl). In this research, these compound was considered in the high temperature phase of cubic bulk system, in which the role of organic cation was investigated in the cubic crystal structure. A preferential orientation of cation align along the $[111]$, the $[101]$ and the $[011]$ directions was also examined in the unit cell. The DFT calculation of electronic structures demonstrated that the orientation of $[011]$ have a characteristic of indirect bandgap, whereas both of $[101]$ and $[111]$ orientations have a direct bandgap. Moreover, the emergence of large anisotropic spin splitting was also found for the $[011]$, $[101]$ and $[111]$ directions, respectively. The first principle calculations of spin polarization revealed a distinct characteristic of spin texture for each orientation. In the case of $[111]$ and $[101]$ directions, Rashba effect was identified with the out-of-plane component whereas Rashba-Dresselhaus effect was also identified with the out-of-plane component in which the spin texture is dominated by Dresselhaus-effect, respectively. On the other hand, in the case of $[011]$ directions, a novel effect exhibiting unidirectional out-of-plane component was achievable called as a Persistent Spin Helix (PSH) states. In order to scrutinize the characteristic of anisotropic spin splitting for each orientation of organic cation, an effective Hamiltonian from group theoretical analysis and symmetry consideration was constructed based on $\vec{k} \cdot \vec{p}$ perturbation theory. Finally, a large spin orbit strength from these effect was calculated and the spin texture model for each orientation was also described with both of the point group C_{3v} and C_s. These findings showed that the high temperature phase of bulk system from the HOIP $CH_3NH_3PbX_3$, is promising material for the development of perovskite-based spintronic devices.

Kata-kata kunci :Hybrid Organic-Inorganic Perovskite, Spin-Orbit Interaction, Rashba-Dresselhaus Effect, Persistent Spin Helix, $\boldsymbol{k \cdot p}$ Perturbation Theory, Density Functional Theory, Spintronic